International Journal of Pure and Applied Researches http://ijopaar.com; 2017 Vol. 4(1); pp. 57-68, ISSN: 2455-474X

# Comparative Analysis of One-Pot Facile Synthesis of Biologically Relevant Novel Tetrahydro-4H-Chromene-3-Carbonitrile and their X-Ray Crystallographic Behaviors

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**Abstract**

*Syntheses and X-ray structural investigations have been compared for the three tetrahydro-4H-chromene-3-carbonitrile derivatives, 2-Amino-4-(3-bromophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (I), 2-Amino-7,7-dimethyl-4-(4-nitrophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile (II) and 2-Amino-7,7-dimethyl-5-oxo-4-(pyridin-4-yl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile hemihydrate (III) respectively. The compounds (I) and (III) crystallize in the monoclinic crystal system with space group $C_2/c$ and compound (II) with space group P-1 crystallizes in the triclinic crystal system. The cyclohexene ring in all the compounds adopts sofa conformation. The pyran ring in compounds (I and II), deviates significantly from planarity and adopts boat conformation while the pyran ring in compound-III is almost planar. In the crystal structure of (I), (II) and (III), the molecules are linked by an elaborate system of N-H···O and N-H···N hydrogen bonds to generate a chain like construct. The crystal structures of all the three molecules were solved by direct method using single crystal X-ray diffraction data collected at room temperature and refined by full-matrix least-squares procedures. The X-ray crystallographic properties of these synthesized compounds of potential biological interests are compared herein.*

**Keywords:** 4H-Pyran, single crystal, X-ray diffraction, Direct methods, Interactions.

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